

4,4'-Thiodianiline
139-65-1 | DTXSID9021344

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.14

Global applicability domain: Inside

Local applicability domain index: 4.70e-01

Confidence level: 6.17e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2,4-Trimethyl-1,3-pentanediol</div> <div>Measured: 1.00</div> <div>Predicted: 1.47</div>	<div>Image not found</div> <div>2,2-Bis(bromomethyl)-1,3-propanediol</div> <div>Measured: 4.79</div> <div>Predicted: 3.35</div>	<div>Image not found</div> <div>Molinate</div> <div>Measured: 25.7</div> <div>Predicted: 14.8</div>
<div>Image not found</div> <div>4-Isobutylmorpholine</div> <div>Measured: 1.78</div> <div>Predicted: 2.69</div>	<div>Image not found</div> <div>Phenacetin</div> <div>Measured: 30.2</div> <div>Predicted: 3.76</div>	